

Comment on: ‘Single-shot simulations of dynamic quantum many-body systems’

P. D. Drummond¹ and J. Brand²

¹Centre for Quantum and Optical Science, Swinburne University of Technology, Melbourne, Victoria 3122, Australia

²Dodd-Walls Centre for Photonics and Quantum Technology, Centre for Theoretical Chemistry and Physics, New Zealand Institute for Advanced Study, Massey University, Private Bag 102904 North Shore, Auckland 0745, New Zealand

In their recent paper[1], Sakmann and Kasevich study the formation of fringe patterns in ultra-cold Bose gases and claim: ‘Here, we show how single shots can be simulated from numerical solutions of the time-dependent many-body Schrödinger equation.’ It would be remarkable if they had solved this exponentially complex equation. Instead they solve nonlinear equations with the aim to approximate the solution of the Schrödinger equation. The authors proceed to criticize phase-space approaches to simulating quantum dynamics and claim the impossibility of interpreting single trajectories of the truncated Wigner (tW) method as single-shot experimental outcomes. Here we aim to provide relevant context and elaborate why we disagree with the authors’ claims.

The multi-configurational time-dependent Hartree or MCTDHB equations used by the authors are based on a multi-mode expansion[2] that is conjectured to converge to the solutions of the Schrödinger equation when many terms are taken into account. Truncating the expansion with a small number M of modes limits the exponential complexity and makes the problem solvable on a computer. Figure 3 demonstrates the approximate nature of this procedure with $N = 10$ particles but does not vindicate the truncation applied for the other two examples, where different observables are approximated with fewer modes and larger particle numbers. For the collision of attractive condensates with $N = 100$ particles the expansion is truncated after $M = 4$ modes (Fig. 1) and for the fluctuating vortices after $M = 2$ (Fig. 2, $N = 10000$). We do not and cannot know how well the MCTDHB expansion approximates the true solution of the Schrödinger equation in the many-particle regime because reliable convergence criteria are only applicable in very specific cases, convergence control is more difficult for larger particle numbers[3], and proposed error estimation procedures have not been implemented yet[4]. Specifically, the free-space dynamics of attractive con-

densates was recently demonstrated to have a slowly-convergent MCTDHB expansion[3]. It is clear that the MCTDHB wave function is, at best, approximate.

The authors criticize the tW approximation for a subtle reason: For pure states, only Gaussians give exact, positive Wigner distributions. Since the tW distribution is not Gaussian and is positive, so the authors argue, it cannot represent a pure quantum state and hence the single-shot interpretation of Wigner phase space trajectories has to be dismissed.

The flaw in this argument is that, like the MCTDHB approach, the tW approximation is not exact but an approximation. Approximate solutions cannot be expected to obey every theorem holding for the exact result and solutions of the truncated MCTDB equations do not do this either, e.g. with respect to the separation of relative and centre-of-mass motion[3]. The exact Wigner function contains the same information as the wave function. The tW approximation includes the first quantum corrections of a $(1/N)$ expansion, and neglects terms of $\mathcal{O}(1/N^2)$, which can have negative values. Despite this, the tW method[5] is well tested against exact methods and experiment[6]. It gives small errors for quantum correlations when N (the number of particle per mode) is large, provided time-scales are not too long[7].

The Wigner method is known to have marginal distributions that are the probability of quadrature measurements, and this property is independent of the positivity of the total distribution[8]. Because of this, it is ideally suited to single-shot interpretations, provided the corresponding measurements are used. Particle instead of quadrature measurements can be interpreted as approximating single shots in volumes with large mode occupation[9], or discrete types of number-phase Wigner distributions can be constructed[10].

In summary, the authors have only solved the Schrödinger equation with an approximation whose accuracy is unclear. Criticising other approximate approaches as not being exact is hypocritical. A separate question concerns the scientific value of simulating experimental single shots using pure quantum states. By definition they are not reproducible. Quantitative tests of theories can only be performed on reproducible results, e.g. on correlation functions that are obtained by averaging over many observations. In current experiments, these usually involve impure density matrices with finite temperature and particle number variation.

[1] Kaspar Sakmann and Mark Kasevich, “Single-shot simulations of dynamic quantum many-body systems,”

Nature Physics **12**, 451–454 (2016).

[2] Ofir E. Alon, Alexej I. Streltsov, and Lorenz S. Ceder-

- baum, “Multiconfigurational time-dependent Hartree method for bosons: Many-body dynamics of bosonic systems,” *Phys. Rev. A* **77**, 033613 (2008).
- [3] Jayson G. Cosme, Christoph Weiss, and Joachim Brand, “Center-of-mass motion as a sensitive convergence test for variational multimode quantum dynamics,” *Phys. Rev. A* **94**, 043603 (2016).
- [4] Kang-Soo Lee and Uwe R. Fischer, “Truncated many-body dynamics of interacting bosons: A variational principle with error monitoring,” *Int. J. Mod. Phys. B* **28**, 1550021 (2014).
- [5] M. J. Steel, M. K. Olsen, L. I. Plimak, P. D. Drummond, S. M. Tan, M. J. Collett, D. F. Walls, and R. Graham, “Dynamical quantum noise in trapped Bose-Einstein condensates,” *Phys. Rev. A* **58**, 4824–4835 (1998).
- [6] Joel F. Corney, Joel Heersink, Ruifang Dong, Vincent Josse, Peter D. Drummond, Gerd Leuchs, and Ulrik L. Andersen, “Simulations and experiments on polarization squeezing in optical fiber,” *Phys. Rev. A* **78**, 023831 (2008).
- [7] Alice Sinatra, Carlos Lobo, and Yvan Castin, “The truncated Wigner method for Bose-condensed gases: limits of validity and applications,” *J. Phys. B* **35**, 3599–3631 (2002).
- [8] M. Hillery, R. F. O’Connell, M. O. Scully, and E. P. Wigner, “Distribution functions in physics: Fundamentals,” *Phys. Rep.* **106**, 121–167 (1984).
- [9] R. J. Lewis-Swan, M. K. Olsen, and K. V. Kheruntsyan, “Approximate particle number distribution from direct stochastic sampling of the Wigner function,” *Phys. Rev. A* **94**, 033814 (2016).
- [10] M. R. Hush, A. R. R. Carvalho, and J. J. Hope, “Number-phase Wigner representation for efficient stochastic simulations,” *Phys. Rev. A* **81**, 033852 (2010).